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Charge density and magnetic anisotropy of Dy-based single molecule magnet

Jacob Overgaard[1], ShangDa Jiang[2], Cheng Gao[1], Emil Andreasen Klahn[1]
[1]*Department Of Chemistry, Aarhus University, Aarhus, Denmark,* [2]*College of Chemistry and Molecular Engineering, Peking University, Beijing, China*
E-mail: jacobo@chem.au.dk

Single molecule magnets (SMMs) are characterized by the ability to maintain the magnitude and orientation of an externally induced magnetization for an extended period of time, even when the external field has been removed. For this reason, researchers have high hopes that this class of materials will eventually be able to provide the smallest possible memory units, as well as playing a prominent role in the development of molecular spintronics as qubits. SMMs are recognized by at least two main features, one being the presence of a stepped hysteresis curve and the other the appearance of a peak in the frequency-dependent out-of-phase ac susceptibility.[1] However, despite the passing of two decades since their discovery, the factors explaining the emergence as well as the disappearance of this property are not well-understood.

SMMs can broadly be divided in two categories, using either 3d transition metals or lanthanides. The latter have inherently strong spin-orbit coupling and the much weaker ligand field splits the spin-orbit coupled ground multiplet. Attention has recently in broad terms turned towards lanthanide-based SMMs, and in particular Dy(III) is a favorite. In a recent explanation for the action of the lanthanide SMMs,[2] the anisotropy of the 4f charge density cloud is said to hinder the rotation of the magnetic moment. However, this statement hinges on approximate gas-phase atomic calculations of the density in the different electronic configurations of the ground multiplet.

Therefore we decided to determine the experimental charge density distribution in a functioning Dy(III) SMM. The molecule, Dy(dbm)3bpy, is shown in Figure 1, together with the magnetic evidence that this is an acting SMM. Based on 50 keV synchrotron X-ray radiation data measured at 20 K, we have performed a multipole model up to a maximum level of l = 6 using Jana2006.[3] The determination of the EDD when dealing with heavy elements is well-known to us and therefore we were encouraged by the rather low residual density maps (|delta(rho)| < 0.5 eÅ-3).

In addition to providing background information and some pertinent experimental details, this presentation will focus on the distribution of the 4f density and its relation to the magnetic properties.

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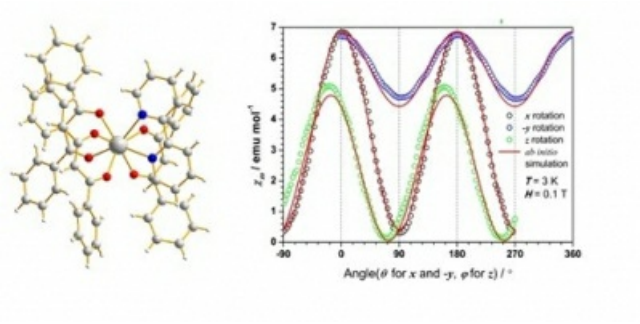

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